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Structural Changes in 2-Acetoxybenzoic Acid (2ABA) in the Presence of Various Solvents: A Quantum Chemical and Spectroscopic Study

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ABSTRACT

2-Acetoxy benzoic acid (2ABA) can produce structural changes in the molecule when dissolved in different solvents depending on factors such as solvent polarity, Hydrogen bonding and solvent interactions. The structural changes of the 2ABA molecule in the presence of solvents were recorded by Fourier Transform Infrared (FT-IR) Spectroscopy in the 4000-0 cm^{-1} range. Additionally, Nuclear Magnetic Resonance (NMR) Spectroscopy was employed to examine changes in chemical shift values associated with the dissolution of the molecule. In another phase of the study, the geometric parameters of the optimized molecules, atomic charges, intensities of the vibrational bands, and vibrational frequencies were calculated using Density Functional Theory (DFT). These calculations were performed at the DFT/B3LYP level with the LanL2DZ basis set, providing a detailed analysis of solvent effects at the molecular level. This study offers significant insights into the interactions of solvent environments with molecular structures and contributes to potential drug development processes.

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1. INTRODUCTION

Different solvents have profound and often unpredictable effects on molecular structures. These effects can drastically change the physical and chemical properties of molecules. Properties of solvents such as polarity, hydrogen bonding capacity and molecular interactions have effects on the electronic structure of 2-Acetoxybenzoic acid (2ABA) [1]. 2ABA is an important organic compound known as acetylsalicylic acid or aspirin [2, 3]. This compound is known for its anti-inflammatory, analgesic, antipyretic and anticoagulant effects. It is also a very important drug as it is widely recommended for various pain conditions such as toothache and menstrual pains [4, 5]. Thus, it is considered as an indispensable drug in medicine due to its versatile use and effective mechanism. 2ABA is a widely used organic compound and is known for its anti-inflammatory and analgesic properties [6]. The molecule contains a benzene ring, an ester group (-$COOCH_3$) and an acetyl group. Structural changes were recorded by quantum chemical calculations using Gaussian 9W software and Fourier Transform Infrared (FT-IR) Spectroscopy. In addition, the changes in chemical shift values were analysed by Nuclear Magnetic Resonance (NMR) Spectroscopy. Calculations using Density Functional Theory (DFT) were carried out at the DFT/B3LYP level and with the LanL2DZ basis set. This study is an important step in understanding the solubility properties and solvent interactions of 2ABA at the molecular level and has the potential for the applicability of this information in drug design and development processes.

The solubility of molecules and their interactions with solvents can lead to significant changes in their structural, electronic and chemical properties. This is a factor that plays an important role in drug development processes [7]. By using DFT to calculate the geometric parameters, atomic charges and vibrational frequencies of the molecule, it is easier to understand the electronic properties of the molecule. Analyzing how chemical shifts change in solvents with NMR spectroscopy can theoretically model the binding and interaction mechanisms of drugs without the need for experimental processes. Thus, it is valuable for designing molecules with desired properties and predicting the effects of changes in molecular structure.

This study shows how 2ABA interacts with various solvents and how these interactions are explained at the molecular level, providing critical information on the solubility, bioavailability and stability of the molecule.

2. MATERIAL AND METHOD

GaussView 6.0.16 programme was used to draw the molecular structures of 2ABA molecule when dissolved in ethanol and water solvents [11]. Quantum chemical calculations of the molecules were performed with Gaussian 09: AS64L-G09RevD.01 programme [12]. DFT and HF approaches were used in the calculations. These calculations were performed at the DFT/B3LYP level with the LanL2DZ basis set and provided a detailed analysis of solvent effects at the molecular level. To study the band structure of the optimised data of the molecules, density of state (DOS) cards were examined with the GaussSum 3.0 tool [13]. The molecular trajectory data were mixed with Gauss's HOMO-LUMO diagram curves.

3. RESULTS AND DISCUSSIONS

Geometry Optimization

Geometric optimisation of the 2ABA molecule and its dissolution in different solvents was performed to find the lowest energy conformation. Gaussian 09: AS64L-G09RevD.01 [12] package programme was used to optimise the bond lengths and angles between the atoms forming the molecule and to adjust the molecule to its most stable state. Fig.1(a) shows the basic structure of the 2ABA molecule without the influence of solvents. Fig.1(b) and 1(c) show the optimised state of the molecule upon dissolution in ethanol and water solvents, respectively. In Fig.1(a) the 2ABA molecule has been optimised without solvent molecules in order to study its individual properties. This structure is necessary to describe a situation where it is free from complex interactions, often referred to as an isolated molecule structure. When 2ABA is optimised in ethanol solvent, interactions with ethanol molecules cause changes in bond angles or lengths due to solvent effects such as hydrogen bonds or Van der Waals forces [7-10]. It shows the optimised structure of 2ABA in water solvent. Water is a highly polar solvent compared to ethanol. It can form strong hydrogen bonds with the carboxyl (-COOH) and ester (-COOR) groups of 2ABA. Therefore, more pronounced changes in structure are observed due to the formation of hydrogen bonds compared to ethanol.

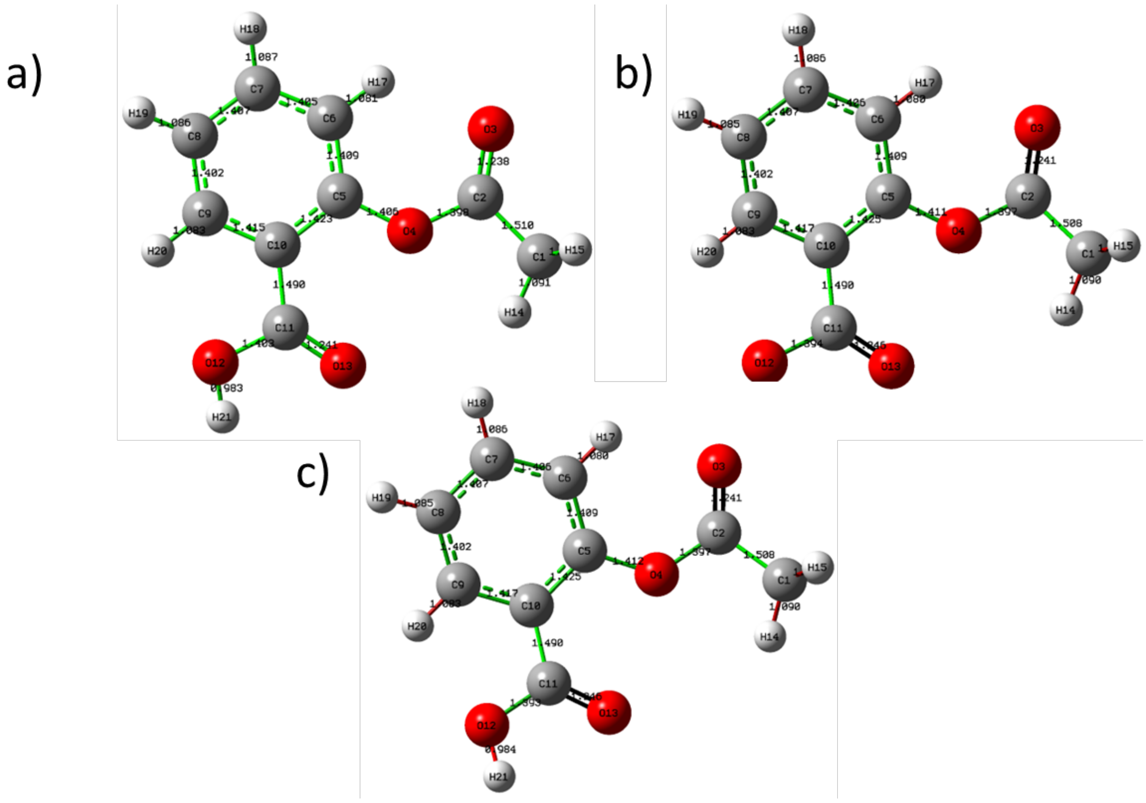

Figure 1. Optimized structure and Bond Lengths of Color Range of **(a)** 2-Acetoxybenzoic Acid, **(b)** Ethanol Solvent, **(c)** Water Solvent

Table 1. Initial Parameters (Angstroms and Degrees)

2-Acetoxybenzoic Acid			2-Acetoxybenzoic Acid-Ethanol			2-Acetoxybenzoic Acid-Water		
Name	**Definition**	**Length (Å)**	**Name**	**Definition**	**Length (Å)**	**Name**	**Definition**	**Length (Å)**
R1	R(1,2)	1.5098	R1	R(1,2)	1.5076	R1	R(1,2)	1.5075
R2	R(1,14)	1.0905	R2	R(1,14)	1.0898	R2	R(1,14)	1.0898
R3	R(1,15)	1.0962	R3	R(1,15)	1.096	R3	R(1,15)	1.096
R4	R(1,16)	1.0962	R4	R(1,16)	1.096	R4	R(1,16)	1.096
R5	R(2,3)	1.2381	R5	R(2,3)	1.2413	R5	R(2,3)	1.2414
R6	R(2,4)	1.3983	R6	R(2,4)	1.3969	R6	R(2,4)	1.3968
R7	R(4,5)	1.4058	R7	R(4,5)	1.4113	R7	R(4,5)	1.4116
R8	R(5,6)	1.4092	R8	R(5,6)	1.4089	R8	R(5,6)	1.4089
R9	R(5,10)	1.4233	R9	R(5,10)	1.4249	R9	R(5,10)	1.425
R10	R(6,7)	1.4055	R10	R(6,7)	1.4061	R10	R(6,7)	1.4061
R11	R(6,17)	1.081	R11	R(6,17)	1.0801	R11	R(6,17)	1.08
R12	R(7,8)	1.4066	R12	R(7,8)	1.4065	R12	R(7,8)	1.4065
R13	R(7,18)	1.0871	R13	R(7,18)	1.0864	R13	R(7,18)	1.0864
R14	R(8,9)	1.4018	R14	R(8,9)	1.4017	R14	R(8,9)	1.4017
R15	R(8,19)	1.0861	R15	R(8,19)	1.0855	R15	R(8,19)	1.0854
R16	R(9,10)	1.4153	R16	R(9,10)	1.4168	R16	R(9,10)	1.4169
R17	R(9,20)	1.0833	R17	R(9,20)	1.0829	R17	R(9,20)	1.0829
R18	R(10,11)	1.4896	R18	R(10,11)	1.4896	R18	R(10,11)	1.4896
R19	R(11,12)	1.4027	R19	R(11,12)	1.3935	R19	R(11,12)	1.393
R20	R(11,13)	1.2414	R20	R(11,13)	1.2461	R20	R(11,13)	1.2463
R21	R(12,21)	0.9835	R21	R(12,21)	0.9842	R21	R(12,21)	0.9843

Frontier Molecular Orbital Analysis (FMO)

The energy gap between the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) is related to the transport of charges in molecules [14]. Molecular orbital arrangement and energy state diagram obtained by dissolving 2ABA molecule in water and ethanol solvents are shown in Fig.2. The energy difference (ΔE) between HOMO and LUMO can affect the reactivity and electronic properties of molecules in solvent environment [15, 16]. The energy difference between HOMO and LUMO of the 2ABA molecule in its pure form (without the addition of any solvent) is 5.093 eV. The change in HOMO and LUMO energies depending on the polarity of solvents such as ethanol and water indicates that solvent molecules interact with the 2ABA molecule and change its electronic structure. A decrease in the HOMO-LUMO energy difference indicates that the molecule becomes more reactive. A lower energy difference means that the energy required for an electron to move from HOMO to LUMO is less. Polar solvents can change the electron distribution of a molecule due to their effect on its chemical reactivity and electronic behavior. The dielectric constant of solvents can affect molecular interactions in solution. Solvents with high dielectric constant affect electron distribution and energy levels at the molecular level by stabilizing the electron cloud of the molecule. However, the use of acid can affect the HOMO and LUMO energy levels by changing the protonation state of the molecule. Protonation changes the electron density, which can lead to changes in molecular orbital energies, thus narrowing the band gap by changing the HOMO and LUMO energies.

The quantum chemical descriptors calculated for the 2ABA molecule in different solvents were calculated as in Table 2. These quantum chemical parameters were calculated from the equations of $I=-E_{HOMO}$; $A=-E_{LUMO}$; $\eta = {}^{1}/_{2}\left[{}^{\partial^2 E}/_{\partial^2 N}\right] = {}^{(I-A)}/_{2}$; $\Delta E=E_{HOMO}-E_{LUMO}$; $\mu=-((I+A)/2)$; $\chi=-\mu$; $\omega=\chi^2/2\eta$; $\varepsilon=1/\omega$; $\omega^{+}={}^{(I+3A)^2}/_{16(I-A)}$; $\omega^{-}={}^{(3I+A)^2}/_{16(I-A)}$. Here, various parameters such as energy difference (ΔE), ionization potential (I), electron affinity (A), electronegativity (χ), chemical hardness (η), nucleophilicity (ε), electrophilicity (ω), dipole moment (μ), and chemical softness (σ) were calculated.

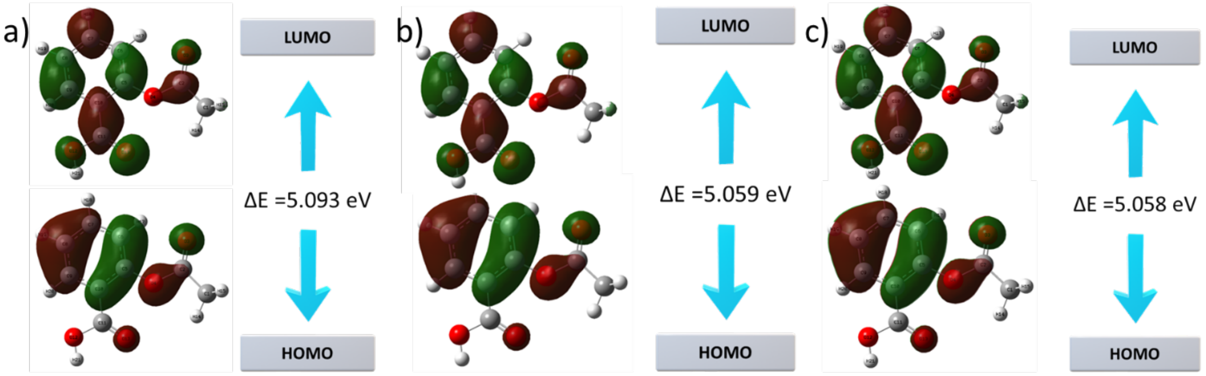

Figure 2. The molecular orbital arrangement and energy state diagram of **(a)** 2-Acetoxybenzoic Acid, **(b)** Ethanol Solvent, **(c)** Water Solvent

Table 2. The calculated quantum chemical descriptors for a) 2-Acetoxybenzoic Acid, b) Ethanol Solvent, c) Water Solvent

Compound	2-Acetoxybenzoic Acid	Ethanol Solvent	Water Solvent
E_{HOMO} (eV)	-7.109	-7.196	-7.202
E_{LUMO} (eV)	-2.016	-2.137	-2.144
ΔE (eV)	5.093	5.059	5.058
η (eV)	2.546	2.529	2.529
σ (eV^{-1})	0.392	0.395	0.395
χ (eV)	4.562	4.666	4.673
μ (eV^{-1})	-4.562	-4.666	-4.673
ω	4.087	4.304	4.317
ε	0.244	0.232	0.231
ω^{+}	0.013	0.007	0.007
ω^{-}	4.576	6.953	6.969

Vibrational Spectroscopic Analysis Spectrum

Vibrational Spectroscopic Analysis describes the peak values at the points where the molecule absorbs the beam when infrared light is incident on the molecule [17]. The position, amplitudes and shapes of these peaks are influenced by many factors such as the molecular structures of the solvent and solute, bond types and interactions in solution [7]. Fig.3 shows the vibrational spectroscopic analysis spectrum of the molecular structures of 2ABA pure molecule in ethanol and water solvents. This graph represents the variation of percent transmittance as a function of wave number (cm^{-1}). The peaks identify the modes of vibration in the molecules of each substance, and as the molecules absorb infrared radiation at certain frequencies, significant decreases in transmittance are observed.

In the pure 2ABA molecule, the peak around 1700 cm^{-1} is due to the C=O stretching for the carboxylic acid group. In the ethanol molecule, peaks were found for the vibrations of both the alcoholic -OH group and the C-H and C-O bonds. The O-H stretching vibration was generally around 3300 cm^{-1}. C-H stretching vibrations are usually located around 2900 cm^{-1}. The water molecule has characteristic peaks due to O-H stretching and bending vibrations. The IR spectrum of pure water usually shows a broad O-H stretching band, which is concluded to lie between about 3200 cm^{-1} and 3500 cm^{-1}.

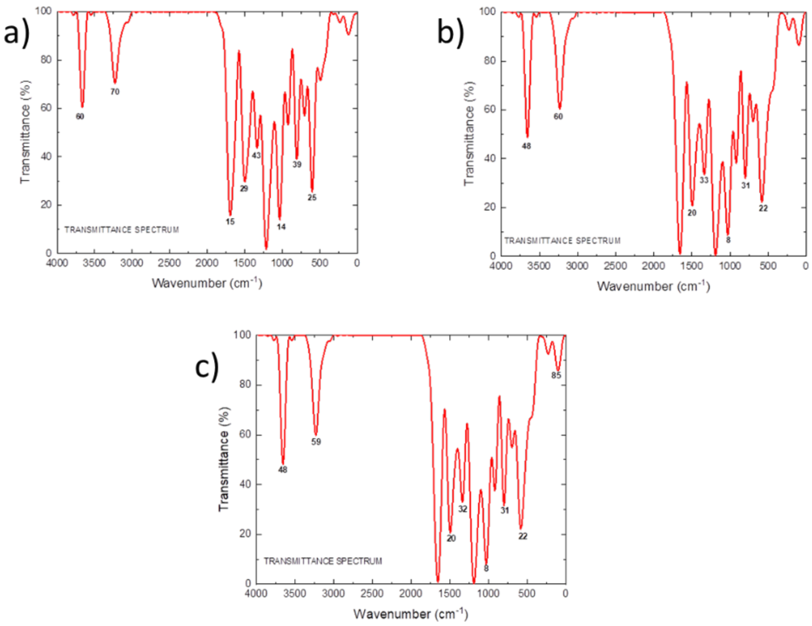

Figure 3. Vibrational Spectroscopic Analysis Spectrum of **(a)** 2-Acetoxybenzoic Acid, **(b)** Ethanol Solvent, **(c)** Water Solvent

Nuclear Magnetic Resonance Spectroscopy

NMR spectroscopy is a method used to study the structural and dynamic properties of molecules. The peaks in the spectrum are based on the behavior of the atomic nuclei in the sample in a magnetic environment and these peaks provide information about the chemical structure of the molecules [18, 19]. The NMR spectra in the graph shown in Fig.4 compare the behavior of the 2ABA molecule in different solvents. Narrow and prominent peaks in the spectrum indicate a dissolved solid sample, while broad and low intensity peaks may indicate high mobility of the molecules or that they have various interactions. Changes between spectra in the direction indicated by the arrows may indicate changes in reaction conditions or time-dependent molecular changes. Looking at the molecular structure pictures, we can see that there can be different types and numbers of molecules. Fig.4(a) represents the NMR spectrum of the pure form of the 2ABA molecule. The spectrum shows the characteristic peaks of hydrogen atoms in various chemical environments of the molecule. In the pure state, the spectrum has clear and sharp peaks, indicating that intermolecular interactions are limited. In Fig.4(b), when the 2ABA molecule is dissolved in ethanol, some changes are noticeable as a result of interaction with ethanol molecules. The polar character of ethanol and its ability to form hydrogen bonds can change the local electronic environment of the hydrogen atoms of the 2ABA molecule. This can lead to changes in the chemical displacement values in the spectrum. These changes observed in the spectrum are an indication of the effect of the solvent on the molecule. In Fig.4(c), water can form stronger hydrogen bonds with 2ABA since it is a more polar solvent than ethanol. These interactions can create even more pronounced changes in the peaks in the spectrum. When dissolved in water, the hydrogen atoms of the 2ABA molecule interact with water molecules, leading to differences in chemical displacements. In particular, the presence of hydrogen bonds in water can result in broader peaks with lower field intensity in the spectrum. Chemical shifts of 2ABA and other solvents are given in Table 2. These shifts give information about the electronic environment around certain atoms in the molecule due to solvent effects.

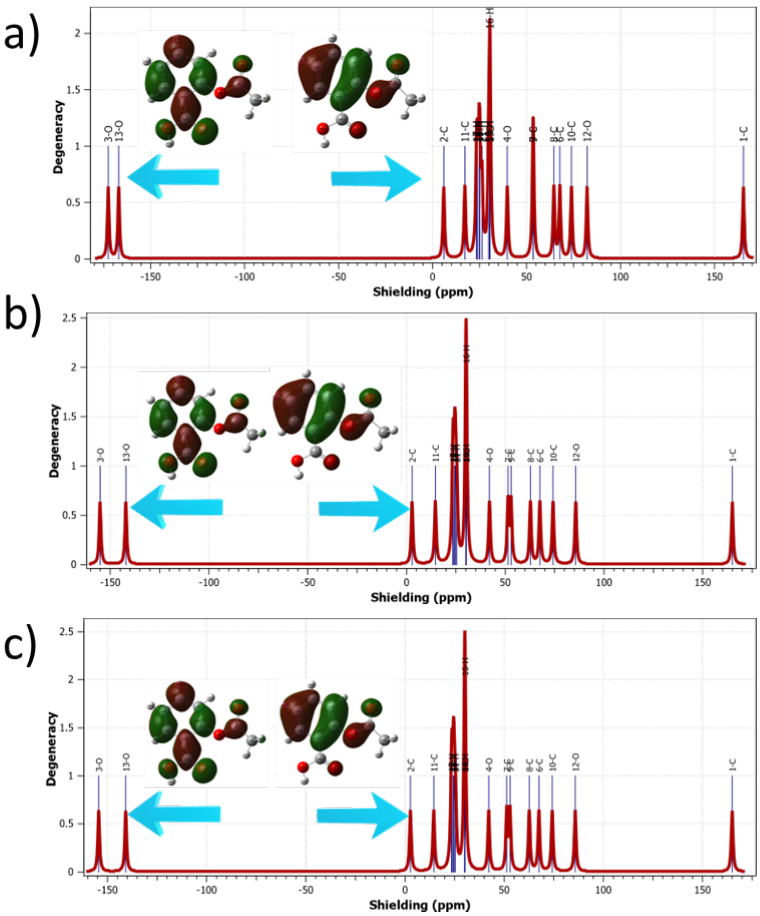

Figure 4. Nuclear Magnetic Resonance Spectroscopy of **(a)** 2-Acetoxybenzoic Acid, **(b)** Ethanol Solvent, **(c)** Water Solvent

Table 3. Chemical shifts of 2ABA molecule and other solvents

2-Acetoxybenzoic Acid		Ethanol Solvent		Water Solvent	
Method	**Shielding (ppm)**	**Method**	**Shielding (ppm)**	**Method**	**Shielding (ppm)**
3-O	-172.557	3-O	-155.1567	3-O	-154.4313
13-O	-166.9776	13-O	-142.0971	13-O	-140.8202
2-C	5.944	2-C	2.8224	2-C	2.7189
11-C	17.1643	11-C	14.6197	11-C	14.4916
17-H	23.3692	17-H	23.4025	17-H	23.4042
20-H	23.8333	20-H	23.7518	20-H	23.7476
18-H	24.771	18-H	24.4376	18-H	24.4215
19-H	25.0911	19-H	24.7445	19-H	24.727
21-H	26.2905	21-H	25.4683	21-H	25.4296
14-H	29.7728	14-H	30.0405	14-H	30.0568
15-H	30.4322	15-H	30.1745	15-H	30.1615
16-H	30.4322	16-H	30.1745	16-H	30.1615
5-C	30.5592	5-C	30.2924	5-C	30.2808
4-O	39.7577	4-O	42.0427	4-O	42.2163
7-C	53.4651	7-C	51.4205	7-C	51.3152
9-C	53.5627	9-C	52.9863	9-C	52.9586
8-C	64.5582	8-C	62.7535	8-C	62.6565
6-C	67.7218	6-C	67.535	6-C	67.5267
10-C	73.8854	10-C	74.2111	10-C	74.232
12-O	82.196	12-O	85.7133	12-O	85.8418
1-C	165.3545	1-C	164.9763	1-C	164.9542

The shift in values from pure compound to solvents indicated the interaction of these oxygen atoms with solvent molecules. Since they are less vulnerable in ethanol and water, it indicates that they form hydrogen bonds with the solvent, which effectively increases the electron density around these atoms. Carbon atoms (2-C, 11-C, 5-C, 7-C, 9-C, 8-C, 6-C, 10-C, 1-C) show different degrees of chemical shift changes in the transition from pure 2ABA to solution. The general trend is for lower ppm values in ethanol and water, indicating increased conservation, possibly due to solvent-solution interactions. Solvents may act as a shield against the external magnetic field, shifting chemical shifts towards the upfield. The significant non-shielding observed for 12-O in the presence of ethanol and water compared to pure matter may indicate a strong interaction with the solvent, possibly hydrogen bonding.

UV–Visible Analysis

UV-Visible spectroscopy is an analysis method that measures how molecules absorb ultraviolet and visible light [20]. This type of spectral analysis is used to obtain information about the structural properties of molecules, their electronic properties and their interactions with solvents. The peaks in each spectrum represent the ability of the substance to absorb light at specific wavelengths [21]. The UV-Visible spectroscopic analyses presented in Fig. 5 show the absorbance spectra of the 2ABA molecule and two different solvents (ethanol and water).

In Fig.5(a), there are prominent peaks showing the transitions between different electronic energy levels of the 2ABA molecule. These peaks are due to π-π* and n-π* electronic transitions in various parts of the molecule. Fig. 5(b) shows that the UV-Visible spectrum of ethanol generally has lower absorbance values. This is because the ethanol molecule has a weak absorbance under UV light. In Fig.5(c), the molecule in water solvent generally shows very low absorbance under UV light. In this case, the peaks in the spectrum may again be due to the electronic transitions of the 2ABA molecule in water. The differences in the spectrum of water solvent compared to ethanol solvent may indicate that the molecular interactions change depending on the solvent. Table 4 shows the peak information of the 2ABA molecule and other solvents.

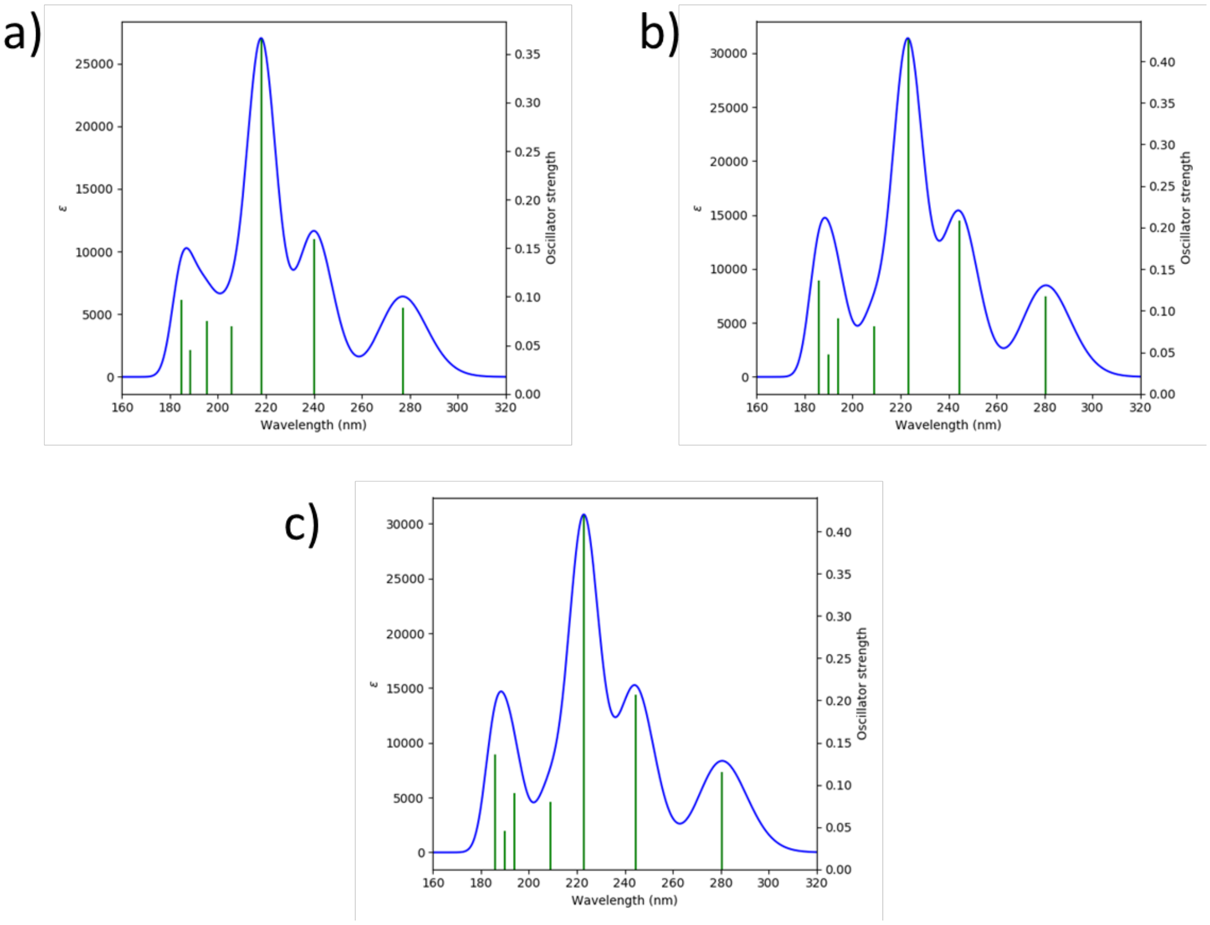

Figure 5. UV–Visible analysis of **(a)** 2-Acetoxybenzoic Acid, **(b)** Ethanol Solvent, **(c)** Water Solvent

Table 4. Peak information of 2ABA and other solvents

2-Acetoxybenzoic Acid		**Ethanol Solvent**		**Water Solvent**	
Wavelength (nm)	**Strength**	**Wavelength (nm)**	**Strength**	**Wavelength (nm)**	**Strength**
291.37	131.282865	285.6	257.3973369	285.29	257.0153244
277.06	116185.3355	280.62	150448.7434	280.61	147912.3192
252.82	131.282865	249.77	257.3973369	249.61	257.0153244
240.29	208871.0382	244.54	268594.121	244.52	265753.8454
227.53	0	224.27	0	224.11	0
218.26	479838.8716	223.12	549414.6156	223.03	538832.6275
212.58	131.282865	208.85	104245.9214	208.91	102806.1297
205.84	90847.74258	208.57	128.6986684	208.37	128.5076622
195.53	98855.99734	194.12	117373.1856	193.97	116556.4496
189.94	0	189.82	60359.6755	189.84	58470.98629
188.6	58814.72352	186.89	0	186.74	0
184.82	127081.8133	185.88	175030.1891	185.84	174384.8976

4. DISCUSSION

In the comparative NMR analysis, important findings on the behavior of the 2ABA molecule in different solvents were obtained. The changes in chemical displacements from the pure state into ethanol and water are a reflection of the interactions of the solvents on the molecule. The changes in ethanol solution were less pronounced, but more pronounced in water due to the higher polarity and stronger hydrogen bonding capacity of water than ethanol. These findings are important for the study of solvent-solvent interactions of the 2ABA molecule and for understanding how these interactions occur at the molecular level. In all three cases, intense absorbance peaks, especially in the UV region (around 200 nm), are striking. This indicates that the 2ABA molecule has strong electronic transitions at these wavelengths, and these transitions can often be due to the aromatic ring of the molecule or chromophore groups such as carbonyl. It is anticipated that the spectral data obtained will contribute to a deeper understanding of the structural and solubility properties of the molecule.

Competing interests

The authors declare that they have no competing interests.

REFERENCES

[1] Manikandan, P., Kumar, M., Chithra, S., Jeelani, A., Khaled, J. M., Abbas, G., & Muthu, S. (2023). Molecular structure solvent–solute, electronic, topology and dynamics simulation studies on 2-[[1-(cyclopropyl methoxy)-4-hydroxy-2-oxoquinoline-3-carbonyl] amino] acetic acid-an effective CKD drug. Journal of Molecular Liquids, 391, 123251.

[2] Toader, A. M., Zarić, S. D., Zalaru, C. M., & Ferbinteanu, M. (2020). The structural details of aspirin molecules and crystals. Current Medicinal Chemistry, 27(1), 99-120.

[3] Govindasamy, P., Gunasekaran, S., & Srinivasan, S. (2014). Molecular geometry, conformational, vibrational spectroscopic, molecular orbital and Mulliken charge analysis of 2-acetoxybenzoic acid. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 130, 329-336.

[4] Grosser, T., Smyth, E., & FitzGerald, G. A. (2011). Anti-inflammatory, antipyretic, and analgesic agents; pharmacotherapy of gout. Goodman and Gilman's the pharmacological basis of therapeutics, 12, 959-1004.

[5] Joshi, M. J. (2013). Study of 2-acetoxybenzoic acid (aspirin) nanoparticles containing w/o microemulsion Kaushal B. Mehta, Bhoomika V. Jogiya, Sonal R. Vasant, Poorvesh M. Vyas and. Archives of Physics Research, 4(4), 14-19.

[6] Schrör, K. (2016). Acetylsalicylic Acid. Almanya: Wiley.

[7] Tanış, E. (2022). New optoelectronic material based on biguanide for orange and yellow organic light emitting diode: A combined experimental and theoretical study. Journal of Molecular Liquids, 358, 119161.

[8] Öztürk, S. T., Aksu, P., Turan, N., Buldurun, K., Tanış, E., & Çolak, N. (2021). Preparation, spectral characterization, ESR measurements and DFT calculations of Schiff base copper (II) complex. Inorganic and Nano-Metal Chemistry, 51(11), 1546-1552.

[9] Çankaya, N., Korcan, S. E., Turan, N., Aydin, B., & Tanış, E. (2023). First report of the synthesis, characterization, DFT calculations of the new oxoethyl methacrylate and o-acetamide and evaluation of antimicrobial, antibiofilm and antioxidant effect. Polycyclic Aromatic Compounds, 43(6), 5139-5157.

[10] Nasidi, I. I., Tanış, E., Kaygili, O., Naeem, S., Majid, A., Mehnen, B., & Bulut, N. (2024). Tailoring the optical and spectroscopic properties of ascorbic acid via solvation with DMSO: A theoretical study using different quantum models. Chemical Physics Impact, 8, 100429.

[11] Dennington R.D., Keith T.A., Millam J.M., GaussView 6.0. 16, Semichem. Inc., Shawnee Mission KS, 2016.

[12] Frisch M.J., Trucks G.W., Schlegel H.B., Scuseria G.E., Robb M.A., Cheeseman J.R., Nakatsuji H., Gaussian09 Revision D. 01, Gaussian Inc.,Wallingford CT, 2009. http://www.gaussian.com.

[13] O'boyle, N.M., Tenderholt, A.L. and Langner, K.M. cclib: A library for package-independent computational chemistry algorithms. J. Comput. Chem. 2008 29: 839-845.

[14] Govindasamy, P., Gunasekaran, S., & Srinivasan, S. (2014). Molecular geometry, conformational, vibrational spectroscopic, molecular orbital and Mulliken charge analysis of 2-acetoxybenzoic acid. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 130, 329-336.

[15] Taniş, E. (2022). A study of silicon and germanium-based molecules in terms of solar cell devices performance. Turkish Journal of Chemistry, 46(5), 1607-1619.

[16] Tanış, E. (2022). Study of electronic, optoelectronic and photonic properties of NBB material in solvent environments. Journal of Electronic Materials, 51(9), 4978-4985.

[17] Cameron, J. M., Bruno, C., Parachalil, D. R., Baker, M. J., Bonnier, F., Butler, H. J., & Byrne, H. J. (2020). Vibrational spectroscopic analysis and quantification of proteins in human blood plasma and serum. In Vibrational Spectroscopy in Protein Research (pp. 269-314). Academic Press.

[18] Nerli, S., McShan, A. C., & Sgourakis, N. G. (2018). Chemical shift-based methods in NMR structure determination. Progress in nuclear magnetic resonance spectroscopy, 106, 1-25

[19] Kebiroglu, H., & Yılmaz, M. (2023). Investigation of UV-Visible Absorption Quantum Effects Doped of Norepinephrine, Mg+2 Atom by Using DFT Method. Journal of Physical Chemistry and Functional Materials, 6(2), 145-151. https://doi.org/10.54565/jphcfum.1332113.

[20] Yılmaz, M., & Kebiroglu, H. (2022). Investigation of K-Serotonin Structure Using Nuclear Magnetic Resonance by Quantum Chemical Methods. Journal of Physical Chemistry and Functional Materials, 5(2), 49-55. https://doi.org/10.54565/jphcfum.1201785

[21] Isah Nasidi, İ., & Kebiroglu, H. (2019). A Theoretical Study on Diphenhydramine Molecule. Journal of Physical Chemistry and Functional Materials, 2(2), 48-53.